

# ethyl linalool 1

<b>Inchi:</b>	InChI=1S/C11H22O/c1-5-11(12,6-2)9-7-8-10(3)4/h8,12H,5-7,9H2,1-4H3
<b>InchiKey:</b>	OKANGIKHTABXMV-UHFFFAOYSA-N
<b>Formula:</b>	C11H22O
<b>SMILES:</b>	CCC(O)(CC)CCC=C(C)C
<b>Mol. weight [g/mol]:</b>	170.29

## Physical Properties

Property code	Value	Unit	Source
gf	-20.57	kJ/mol	Joback Method
hf	-323.92	kJ/mol	Joback Method
hfus	19.81	kJ/mol	Joback Method
hvap	55.50	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.284		Crippen Method
mcvol	167.420	ml/mol	McGowan Method
pc	2254.67	kPa	Joback Method
rinpol	1168.90		NIST Webbook
rinpol	1168.90		NIST Webbook
tb	544.07	K	Joback Method
tc	718.97	K	Joback Method
tf	257.93	K	Joback Method
vc	0.640	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.20	J/mol×K	544.07	Joback Method
cpg	427.75	J/mol×K	573.22	Joback Method
cpg	441.56	J/mol×K	602.37	Joback Method
cpg	454.68	J/mol×K	631.52	Joback Method
cpg	467.14	J/mol×K	660.67	Joback Method
cpg	478.98	J/mol×K	689.82	Joback Method
cpg	490.23	J/mol×K	718.97	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R185489&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R185489&amp;Units=SI</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvp:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinp:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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